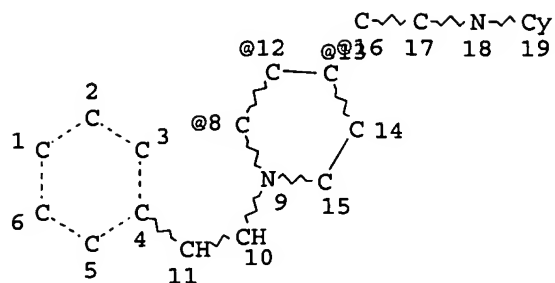


=> d l10

L10 HAS NO ANSWERS

L10 STR



VPA 16-8/12/13 U

NODE ATTRIBUTES:

NSPEC IS C AT 18

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 8 4

NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE

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=> d his l12

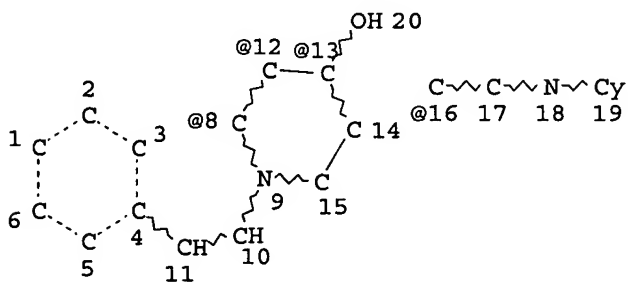
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L12 239 S L10 FUL

=> d l15

L15 HAS NO ANSWERS

L15 STR



VPA 16-8/12/13 U

NODE ATTRIBUTES:

NSPEC IS C AT 18

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 8 4

NUMBER OF NODES IS 19

STEREO ATTRIBUTES: NONE

=> search l15

ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:sss

ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:subset

ENTER SUBSET L# OR (END):l12

ENTER SUBSET SEARCH SCOPE - SAMPLE, FULL, RANGE, OR (END):ful

FULL SUBSET SEARCH INITIATED 10:26:37 FILE 'REGISTRY'

FULL SUBSET SCREEN SEARCH COMPLETED - 206 TO ITERATE

100.0% PROCESSED 206 ITERATIONS

200 ANSWERS

SEARCH TIME: 00.00.01

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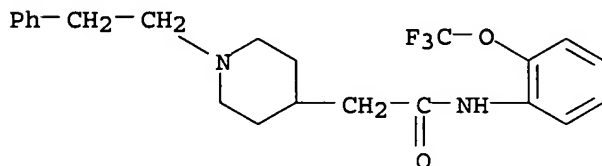
L17 39 L12 NOT L16

=> d scan

L17 39 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 4-Piperidineacetamide, 1-(2-phenylethyl)-N-[2-(trifluoromethoxy)phenyl]-  
(9CI)

MF C22 H25 F3 N2 O2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

41.16

454.60

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

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FILE 'CAPLUS' ENTERED AT 10:26:53 ON 06 SEP 2006

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FILE COVERS 1907 - 6 Sep 2006 VOL 145 ISS 11  
FILE LAST UPDATED: 5 Sep 2006 (20060905/ED)

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<http://www.cas.org/infopolicy.html>

=> s l17

L18 10 L17

=> d his

(FILE 'HOME' ENTERED AT 10:12:19 ON 06 SEP 2006)

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L3 STRUC  
L4 5 S L3  
L5 STRUC  
L6 0 S L5  
L7 234 S L3 FUL  
L8 25 SEARCH L5 SSS SUB=L7 FUL

FILE 'CAPLUS' ENTERED AT 10:18:32 ON 06 SEP 2006

L9 4 S L8

FILE 'REGISTRY' ENTERED AT 10:21:24 ON 06 SEP 2006

FILE 'CAPLUS' ENTERED AT 10:22:11 ON 06 SEP 2006

FILE 'REGISTRY' ENTERED AT 10:22:42 ON 06 SEP 2006

L10 STRUC  
L11 0 S L10  
L12 239 S L10 FUL

FILE 'CAPLUS' ENTERED AT 10:23:44 ON 06 SEP 2006

L13 22 S L12  
L14 18 S L13 NOT L9

FILE 'REGISTRY' ENTERED AT 10:24:40 ON 06 SEP 2006

L15 STRUC  
L16 200 SEARCH L15 SSS SUB=L12 FUL  
L17 39 S L12 NOT L16

FILE 'CAPLUS' ENTERED AT 10:26:53 ON 06 SEP 2006

L18 10 S L17  
L19 6 S L18 NOT L9  
L20 0 S L19 AND (INFLAMM? OR (ANTI(W)INFLAMM?))

=> d bib abs hitstr l19 1-6

L19 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2003:887681 CAPLUS

DN 139:364834

TI Heterocyclic analgesic compounds, namely N-[1-(1-phenethylpiperidin-3-yl)ethyl]-N-phenylpropionamide and analogs, with activity at opioid receptors, and method of use thereof

IN Cuny, Gregory D.; Shao, Liming; Hauske, James R.; Heffernan, Michele L. R.; Aquila, Brian M.; Wu, Xinhe; Wang, Fengjiang; Bannister, Thomas D.

PA Sepracor Inc., USA

SO U.S., 91 pp., Cont.-in-part of U.S. Ser. No. 579,398.

CODEN: USXXAM

DT Patent

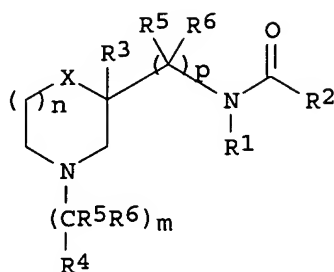
LA English

FAN.CNT 6

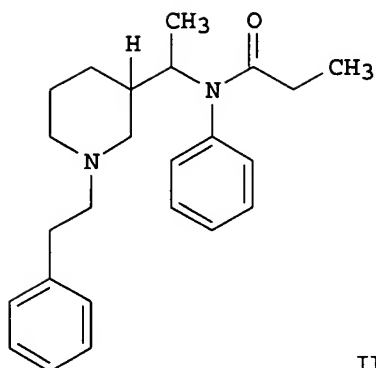
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PI	US 6645980	B1	20031111	US 2000-717174	20001120
	US 6677332	B1	20040113	US 2000-579398	20000525
	US 2002016337	A1	20020207	US 2001-798803	20010302
	US 6635661	B2	20031021		
	US 2003069418	A1	20030410	US 2002-121029	20020411
PRAI	US 2000-579398	A2	20000525		

US 1999-135721P	P	19990525
US 1999-168979P	P	19991203
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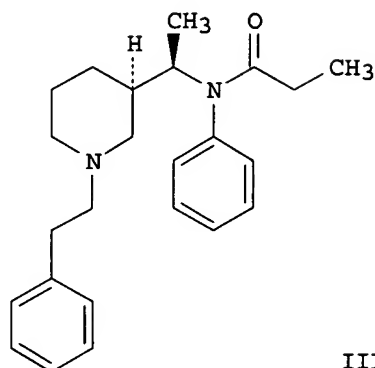
OS MARPAT 139:364834  
GI



I



II



III

AB One aspect of the invention relates to novel heterocyclic compds. (6 Markush structures given), e.g., I [wherein: m = 1, 2, 3 or 4; n = 1 or 2; p = 1 or 2; R1 = alkyl, aryl, heteroaryl, or cycloalkyl; R2 = H, alkyl, fluoroalkyl, aryl, heteroaryl, or cycloalkyl; R1 and R2 may be connected through a covalent bond; R3 = H, alkyl, aryl, OR2, OC(O)R2CH2OR2, or CO2R2; wherein any 2 instances of R3 may be connected by a covalent tether whose backbone consists of 1, 2, 3, or 4 C atoms; R4 = H, alkyl, aryl, heteroaryl, alkenyl, or cycloalkyl; R5 = H, alkyl, CH2Y, aryl, heteroaryl, F, OR2, or OC(O)R2; R6 = H, alkyl, CH2Y, aryl, heteroaryl, F, OR2, or OC(O)R2; Y = OR2, N(R2)2, SR2, S(O)R2, S(O)2R2, or P(O)(OR2)2; a covalent bond may connect R4 and an instance of R5 or R6 that is attached to the C chain between R4 and the ring N explicitly shown; any 2 geminal or vicinal instances of R5 and R6 may be connected through a covalent bond; X = C(R3)2, O, S, SO, SO2, NR2, NC(O)OR2, or C=O; and the stereochem. configuration at any stereocenter is (R)-, (S)-, or mixed]. A second aspect of the invention relates to the use of the compds. as ligands for various cellular receptors, including opiate receptors, other G-protein-coupled receptors, and ion channels. An addnl. aspect of the invention relates to the use of the compds. as analgesics. A large number of synthetic and biol. examples are given, including a combinatorial preparation. For instance, 3-(1-hydroxyethyl)piperidine-1-carboxylic acid tert-Bu ester was converted to its mesylate ester, and this reacted with aniline to give 3-[1-(phenylamino)ethyl]piperidine-1-carboxylic acid tert-Bu ester. Amidation of this with propionyl chloride, deprotection of the BOC group

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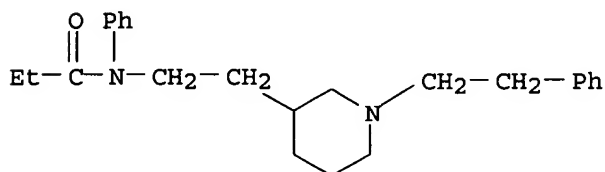
IT 309747-86-2P, N-[2-(1-Phenethylpiperidin-3-yl)ethyl]-N-phenylpropionamide

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of [(phenethylpiperidiny)ethyl]phenylpropionamides and analogs as analgesics)

RN 309747-86-2 CAPLUS

CN Propanamide, N-phenyl-N-[2-[1-(2-phenylethyl)-3-piperidiny]ethyl]- (9CI)  
(CA INDEX NAME)



RE.CNT 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2002:107910 CAPLUS

DN 136:167282

TI Heterocyclic analgesic compounds, namely N-[1-(1-phenethylpiperidin-3-yl)ethyl]-N-phenylpropionamide and analogs, with activity as opioid receptors, and method of use thereof

IN Cuny, Gregory D.; Shao, Liming; Hauske, James R.; Heffernan, Michele L. R.; Aquila, Brian M.; Wu, Xinhe; Wang, Fengjiang; Bannister, Thomas D.

PA Sepracor, Inc., USA

SO U.S. Pat. Appl. Publ., 107 pp., Cont.-in-part of U.S. Ser. No. 717,174.  
CODEN: USXXCO

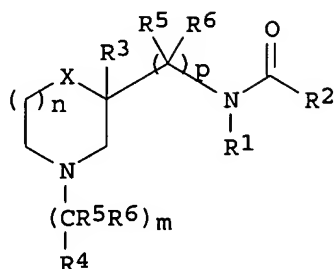
DT Patent

LA English

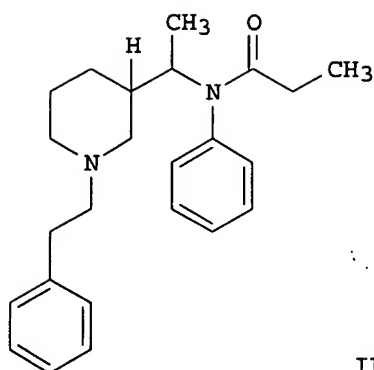
FAN.CNT 6

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	US 6645980	B1	20031111	US 2000-717174	20001120
	WO 2002069895	A2	20020912	WO 2002-US6274	20020301
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RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

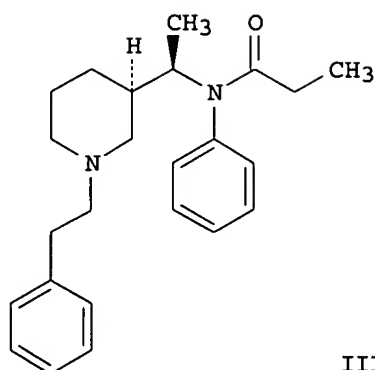
AU 2002306624	A1	20020919	AU 2002-306624	20020301
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US 2000-717174	A2	20001120		
US 1999-135721P	P	19990525		
US 1999-168979P	P	19991203		
US 2000-195809P	P	20000411		
US 2001-798803	A	20010302		
US 2001-284374P	P	20010417		
WO 2002-US6274	W	20020301		
OS MARPAT 136:167282				
GI				



I



II



III

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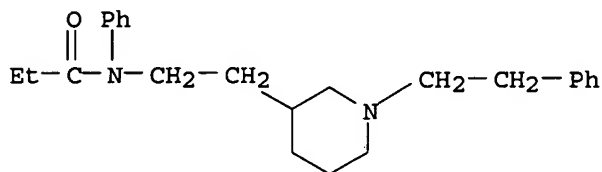
IT 309747-86-2P, N-[2-(1-Phenethylpiperidin-3-yl)ethyl]-N-phenylpropionamide

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of [(phenethylpiperidinyl)ethyl]phenylpropionamides and analogs as analgesics)

RN 309747-86-2 CAPLUS

CN Propanamide, N-phenyl-N-[2-[1-(2-phenylethyl)-3-piperidinyl]ethyl]- (9CI)  
(CA INDEX NAME)



L19 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2001:886067 CAPLUS

DN 136:20020

TI Heterocyclic analgesic compounds, namely N-[1-(1-phenethylpiperidin-3-yl)ethyl]-N-phenylpropionamide and analogs, with activity at opioid receptors, and method of use thereof

IN Cuny, Gregory D.; Shao, Liming; Hauske, James R.; Heffernan, Michele L. R.; Aquila, Brian M.; Wu, Xinhe; Wang, Fengjian; Bannister, Thomas D.

PA Sepracor, Inc., USA

SO PCT Int. Appl., 229 pp.

CODEN: PIXXD2

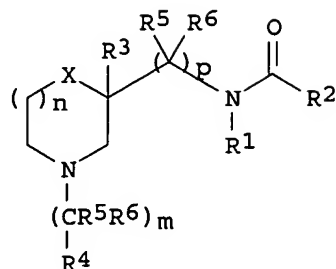
DT Patent

LA English

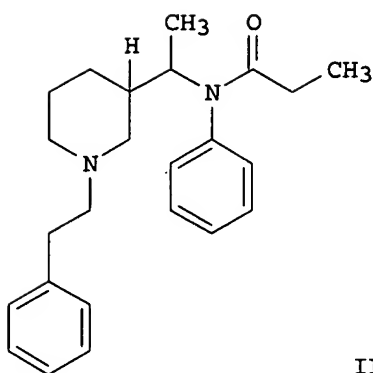
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PRAI	US 2000-579398	A	20000525		
	US 1999-135721P	P	19990525		

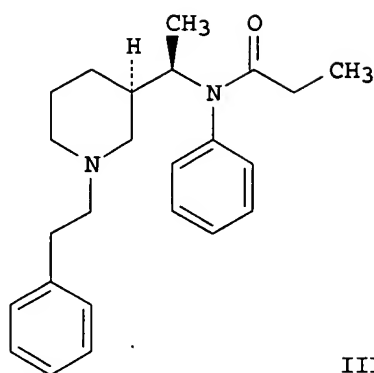




I



II



III

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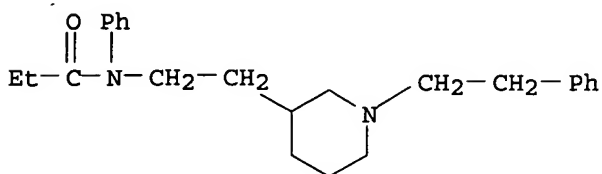
IT 309747-86-2P, N-[2-(1-Phenethylpiperidin-3-yl)ethyl]-N-phenylpropionamide

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of [(phenethylpiperidiny)ethyl]phenylpropionamides and analogs as analgesics)

RN 309747-86-2 CAPLUS

CN Propanamide, N-phenyl-N-[2-[1-(2-phenylethyl)-3-piperidiny]ethyl]- (9CI)  
(CA INDEX NAME)



RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2000:842113 CAPLUS

DN 134:29315

TI Heterocyclic analgesic compounds and methods of use thereof

IN Cuny, Gregory D.; Shao, Liming; Hauske, James R.; Heffernan, Michele L. R.; Aquila, Brian M.; Wu, Xinhe; Wang, Fengjian; Bannister, Thomas D.

PA Sepracor, Inc., USA

SO PCT Int. Appl., 216 pp.

CODEN: PIXXD2

DT Patent

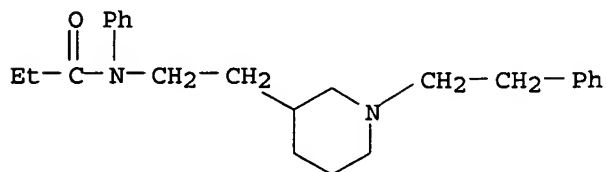
LA English

FAN.CNT 6

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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	R:				
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	JP 2003500392	T2	20030107	JP 2000-619775	20000525
	AU 777760	B2	20041028	AU 2000-52953	20000525
PRAI	US 1999-135721P	P	19990525	6677,332	
	US 1999-168979P	P	19991203		
	US 2000-195809P	P	20000411		
	WO 2000-US14579	W	20000525		
OS	MARPAT 134:29315				

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

- AB The present invention discloses novel nitrogen heterocycles of formula I (A = (CH<sub>2</sub>)<sub>b</sub>, Z = (CH<sub>2</sub>)<sub>y</sub>, W = (CH<sub>2</sub>)<sub>n</sub>, where b = 0 or 1, yr = 1 or 2, and n = 1, 2 or 3 with provisions; X = C(R<sub>3</sub>)<sub>2</sub>, O, S, SO<sub>2</sub>, NR<sub>2</sub>, NCO<sub>2</sub>R<sub>2</sub>, or CO; R<sub>1</sub> = alkyl, aryl, heteroaryl, or cycloalkyl; R<sub>2</sub> = H, alkyl, fluoroalkyl, aryl, heteroaryl, or cycloalkyl; R<sub>1</sub> and R<sub>2</sub> may be connected via covalent bond; R<sub>3</sub> = H, alkyl, aryl, OR<sub>2</sub>, OCOR<sub>2</sub>, CH<sub>2</sub>OR<sub>2</sub>, or CO<sub>2</sub>R<sub>2</sub>, wherein any two instances of R<sub>3</sub> may be connected via divalent carbon bridge; R<sub>4</sub> = H, alkyl, aryl, heteroaryl, alkenyl, or cycloalkyl; R<sub>5</sub> or R<sub>6</sub> = H, alkyl, CH<sub>2</sub>Y, aryl, heteroaryl, F, OR<sub>2</sub> or OCOR<sub>2</sub>; Y = OR<sub>2</sub>, N(R<sub>2</sub>)<sub>2</sub>, SR<sub>2</sub>, SOR<sub>2</sub>, SO<sub>2</sub>R<sub>2</sub> or PO(OR<sub>2</sub>)<sub>2</sub>; R<sub>4</sub> may be covalently attached to an adjacent R<sub>5</sub> or R<sub>6</sub>; p = 1, 2, 3 or 4; m = 0, 1, or 2) and II (y = 1; n = 2; b = 0) as well as methods for preparation. Compound III was prepared by successive amidation of (R)-N-(1-Boc-piperidin-3-ylmethyl)aniline, deprotection and alkylation. Methods employed to prepare claimed compds. included combinatorial chemical providing ninety-six piperidinyll derivs. with IC<sub>50</sub> values (μM) ranging 0.31-5.76 and 0.08-4 against κ and μ opioid receptors, resp. III was five times stronger [ED<sub>50</sub> (μg/kg) <500] than morphine [ED<sub>50</sub> <2500] as an analgesic as demonstrated in a standard rat tail flick test. A second aspect of the present invention relates to the use of the novel heterocyclic compds. as ligands for various cellular receptors, including opiate receptors, other the G-protein coupled receptors, and ion channels. An addnl. aspect of the invention relates to the use of the novel heterocyclic compds. as analgesics.
- IT 309747-86-2P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and biol. activity of nitrogen heterocyclic analgesic compds.)
- RN 309747-86-2 CAPLUS
- CN Propanamide, N-phenyl-N-[2-[1-(2-phenylethyl)-3-piperidinyl]ethyl]- (9CI)  
(CA INDEX NAME)

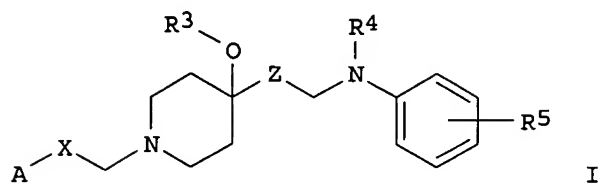


- L19 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2000:742073 CAPLUS
- DN 133:305612
- TI 4-Hydroxypiperidine derivatives as remedies for neuropathic pain
- IN Yamamoto, Ichiro; Itoh, Manabu; Yamasaki, Fumiaki; Akada, Yasushige; Miyazaki, Yutaka; Ogawa, Shinichi
- PA Mochida Pharmaceutical Co., Ltd., Japan
- SO PCT Int. Appl., 127 pp.  
CODEN: PIXXD2
- DT Patent
- LA Japanese
- FAN.CNT 2
- | PATENT NO.    | KIND | DATE     | APPLICATION NO. | DATE     |
|---------------|------|----------|-----------------|----------|
| WO 2000061558 | A1   | 20001019 | WO 2000-JP2332  | 20000410 |
- W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR,

CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU,  
 ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU,  
 LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE,  
 SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA,  
 ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM  
 RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,  
 DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,  
 CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

CA 2369695 AA 20001019 CA 2000-2369695 20000410  
 EP 1182193 A1 20020227 EP 2000-915468 20000410  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
 IE, SI, LT, LV, FI, RO  
 US 2002049229 A1 20020425 US 2001-969644 20011004  
 US 6642257 B2 20031104  
 PRAI JP 1999-103212 A 19990409  
 JP 2000-23116 A 20000131  
 WO 2000-JP2332 W 20000410

GI



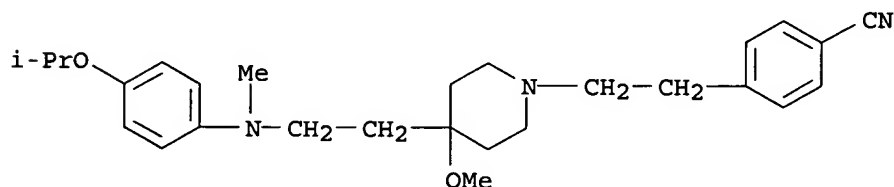
AB Comps. represented by general formula (I) or salts thereof and medicinal compns. containing the same as the active ingredient: wherein A represents, for example, Ph substituted by R1 and R2, unsubstituted furyl or unsubstituted thienyl (wherein R1 represents, for example, hydrogen, fluoro, chloro, trifluoromethyl, nitro, cyano or methyl; and R2 represents, for example, hydrogen); R3 represents, for example, hydrogen or methyl; R4 represents, for example, hydrogen or methyl; R5 represents ethoxy or iso-propoxy; X represents -CH(OH)- or methylene; and Z represents, for example, a single bond or optionally hydroxylated methylene. These compds. can be orally administered as remedies for neuropathic pain and exhibit excellent effect while showing little side effects.

IT 302518-94-1P 302521-71-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (4-hydroxypiperidine derivs. as remedies for neuropathic pain)

RN 302518-94-1 CAPLUS

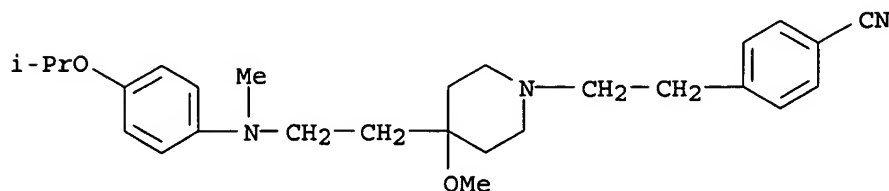
CN Benzonitrile, 4-[2-[4-methoxy-4-[2-[methyl[4-(1-methylethoxy)phenyl]amino]ethyl]-1-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)



RN 302521-71-7 CAPLUS

CN Benzonitrile, 4-[2-[4-methoxy-4-[2-[methyl[4-(1-

methylethoxy)phenyl]amino]ethyl]-1-piperidinyl]ethyl]-, dihydrochloride  
(9CI) (CA INDEX NAME)

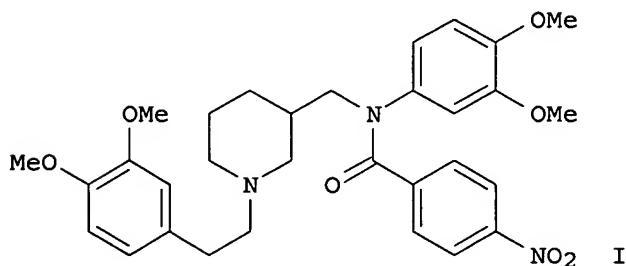


●2 HCl

RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 1996:593888 CAPLUS  
DN 125:221598  
TI Preparation of N-aryl-N-heterocyclylalkyl-4-nitrobenzamides and analogs as  
antiarrhythmics  
IN Nadler, Guy Marguerite Marie Gerard; Souchet, Michel Louis; Legave, Marie  
Noel Genevieve  
PA Smithkline Beecham Laboratoires Pharmaceutiques, Fr.  
SO Fr. Demande, 29 pp.  
CODEN: FRXXBL  
DT Patent  
LA French  
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	FR 2729142	A1	19960712	FR 1995-106	19950106
PRAI	FR 1995-106		19950106		
OS	MARPAT 125:221598				
GI					

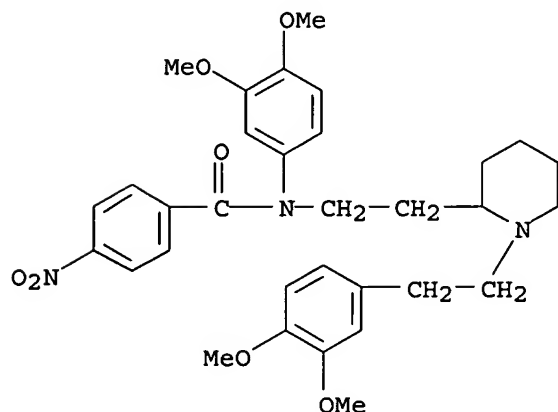


AB R1Z1N(Z2R2)Z4ZZ3R3 [R1 = (un)substituted Ph; R2 = (hetero)aryl,  
arylalk(en)yl, etc.; R3 = (hetero)aryl; Z = N-containing (un)substituted  
heterocyclylene; Z1 = bond, CH2, OCH2CH2, etc.; Z2 = CO, NHCO, SO2, etc.;  
Z3 = alkylene; Z4 = bond or alkylene] were prepared as antiarrhythmics (no  
data). Thus, pyridine-3-carboxaldehyde was condensed with  
3,4-(MeO)2C6H3NH2 and the product converted in 6 steps to title compound I.  
IT 181522-50-9P 181522-52-1P  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological  
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);  
BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of N-aryl-N-heterocyclalkyl-4-nitrobenzamides and analogs as antiarrhythmics)

RN 181522-50-9 CAPLUS

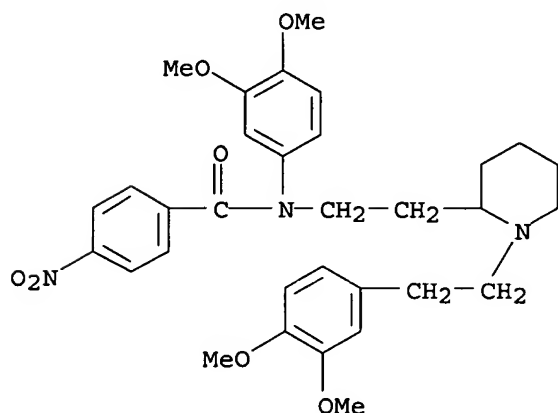
CN Benzamide, N-(3,4-dimethoxyphenyl)-N-[2-[1-[2-(3,4-dimethoxyphenyl)ethyl]-2-piperidinyl]ethyl]-4-nitro-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 181522-52-1 CAPLUS

CN Benzamide, N-(3,4-dimethoxyphenyl)-N-[2-[1-[2-(3,4-dimethoxyphenyl)ethyl]-2-piperidinyl]ethyl]-4-nitro- (9CI) (CA INDEX NAME)



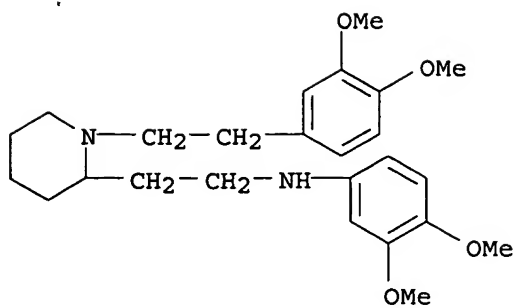
IT 181522-72-5P 181522-74-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of N-aryl-N-heterocyclalkyl-4-nitrobenzamides and analogs as antiarrhythmics)

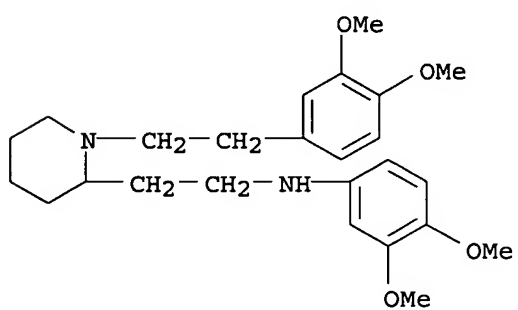
RN 181522-72-5 CAPLUS

CN 2-Piperidineethanamine, N-(3,4-dimethoxyphenyl)-1-[2-(3,4-dimethoxyphenyl)ethyl]- (9CI) (CA INDEX NAME)



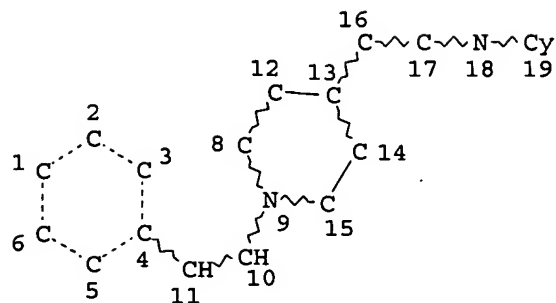
RN 181522-74-7 CAPLUS

CN 2-Piperidineethanamine, N-(3,4-dimethoxyphenyl)-1-[2-(3,4-dimethoxyphenyl)ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

=> d 13  
 L3 HAS NO ANSWERS  
 L3 STR



NODE ATTRIBUTES:  
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 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RSPEC 8 4  
 NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE

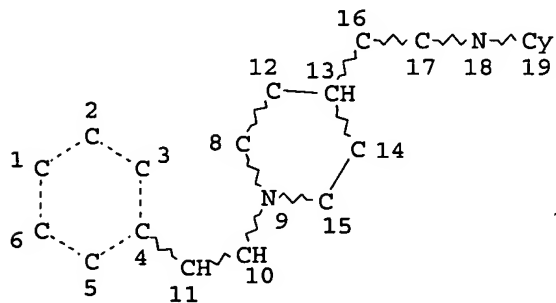
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 FULL SCREEN SEARCH COMPLETED - 75339 TO ITERATE

100.0% PROCESSED 75339 ITERATIONS  
 SEARCH TIME: 00.00.01

234 ANSWERS

L7 234 SEA SSS FUL L3

=> d 15  
 L5 HAS NO ANSWERS  
 L5 STR



NODE ATTRIBUTES:  
 NSPEC IS C AT 18  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RSPEC 8 4  
 NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE



=> search 15

ENTER TYPE OF SEARCH (SSS), CSS, FAMILY, OR EXACT:sss

ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:17

'L7' IS NOT A VALID SEARCH SCOPE

ENTER SCOPE OF SEARCH (SAMPLE), FULL, RANGE, OR SUBSET:subset

ENTER SUBSET L# OR (END):17

ENTER SUBSET SEARCH SCOPE - SAMPLE, FULL, RANGE, OR (END):ful

FULL SUBSET SEARCH INITIATED 10:18:05 FILE 'REGISTRY'

FULL SUBSET SCREEN SEARCH COMPLETED - 234 TO ITERATE

100.0% PROCESSED 234 ITERATIONS

25 ANSWERS

SEARCH TIME: 00.00.01

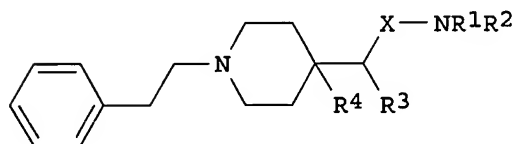
L8

25 SEA SUB=L7 SSS FUL L5

=> d bib abs 19 1-4

L9 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 2003:42107 CAPLUS  
DN 138:89689  
TI Preparation of 1-phenylethylpiperidines as analgesics  
IN Sundermann, Bernd; Hoenen, Lambert; Buschmann, Helmut; Koegel,  
Babette-Yvonne; Friderichs, Elmar  
PA Gruenenthal G.m.b.H., Germany  
SO PCT Int. Appl., 54 pp.  
CODEN: PIXXD2  
DT Patent  
LA German  
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003004026	A1	20030116	WO 2002-EP7379	20020703
	W:			AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM	
	RW:			GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG	
	DE 10132746	A1	20030206	DE 2001-10132746	20010705
	EP 1406623	A1	20040414	EP 2002-745424	20020703
	R:			AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK	
	US 2004171640	A1	20040902	US 2004-751584	20040105
PRAI	DE 2001-10132746	A	20010705		
	WO 2002-EP7379	W	20020703		
OS	MARPAT 138:89689				
GI					



I

AB The title compds. [I; X = CH2, CO; R1 = (substituted) (hetero)aryl; R2 = H, COR5, SO2R5, (substituted) (saturated) (branched) (cyclo)aliphatic group, (hetero)aryl, (hetero)arylalkyl; R3, R4 = H; or R3R4 = bond; R5 = (substituted) (saturated) (branched) (cyclo)aliphatic group, (hetero)aryl, (hetero)arylalkyl], were prepared I showed at 1-10 mg/kg i.v. an antinociceptive effect of 56-100% in the phenylquinone-induced writhing test on mice and at 0.1-1 mg/kg i.v. an antinociceptive effect of 21-56% in the mice tail-flick test.

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 2002:578092 CAPLUS  
DN 138:147171  
TI Electronic-topological study of the structure-activity relationships in a series of piperidine morphinomimetics  
AU Sim, E.; Dimoglo, A.; Shvets, N.; Ahsen, V.

CS Gebze Institute of Technology, Gebze, 41400, Turk.  
SO Current Medicinal Chemistry (2002), 9(16), 1537-1545  
CODEN: CMCHE7; ISSN: 0929-8673

PB Bentham Science Publishers

DT Journal

LA English

AB Structure-activity relationships (SAR) are studied in the series of 4,4-disubstituted piperidine morphinomimetics (42 compds.) by means of the Electronic-Topol. Method (ETM). In the frameworks of this approach, its input data were taken as the results of conformational and quantum-mech. calcns. These calcns. had been carried out for all compds. from the series under study, taking into account their neutral and protonated by the nitrogen of piperidine cycle forms. The ETM application resulted in a set of pharmacophores and anti-pharmacophores, which formed a basis of a system used to predict analgesic activity. First of all, the system was tested on known analgesics. Testing has shown a good agreement with the exptl. data. Then, the system was applied to a few compds. with similar structures but unknown activity. The results of the study could be used for computer screening and design of novel compds. with analgesics properties as new potential drugs.

RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1994:289418 CAPLUS

DN 120:289418

TI Examining structure-activity relationships in a series of piperidine analgesics with an electron topological technique

AU Sim, E. P.; Dimoglo, A. S.

CS Inst. Khim., Kishinev, Moldova

SO Khimiko-Farmatsevticheskii Zhurnal (1993), 27(8), 30-4

CODEN: KHFZAN; ISSN: 0023-1134

DT Journal

LA Russian

AB Mol. mechanics and quantum chemical were used to investigate structure-activity relations in a series of piperidine derivs. which possess morphine-like activity in unspecified laboratory animals. An electron topol. approach was employed. A number of characters were found to correlate with analgesic activity. Structure-activity relations are discussed.

L9 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1983:16551 CAPLUS

DN 98:16551

TI Synthesis and pharmacological studies of 4,4-disubstituted piperidines: a new class of compounds with potent analgesic properties

AU Huegi, Bruno S.; Ebnoether, Anton M.; Rissi, Erwin; Gadiant, Fulvio; Hauser, Daniel; Roemer, Dietmar; Buescher, Heinz H.; Petcher, Trevor J.

CS Preclin. Res., Sandoz Ltd., Basel, CH-4002, Switz.

SO Journal of Medicinal Chemistry (1983), 26(1), 42-50

CODEN: JMCMAR; ISSN: 0022-2623

DT Journal

LA English

OS CASREACT 98:16551

GI For diagram(s), see printed CA Issue.

AB Disubstituted piperidines I [R1 = PhCH2, H, PhCH2CH2, 2-ClC6H4CH2CH2, 4-MeOC6H4CH2CH2, Me, allyl, heptyl; R2 = OH, O2CEt; R3 = H, Me, Bu, CHMe2; R4 = H, Me; R5 = substituted amino; R3R4 = (CH2)2, (CH2)4] were prepared and evaluated for analgesic activity. I show analgesic potency comparable to morphine in the mouse writhing and tail-flick tests. A number of compds. exhibit high affinity for [3H]naloxone binding sites in rat brain membranes. Among the most potent derivs. are I (R1 = 2-ClC6H4CH2CH2, R2 = OH, R3 = Me, R4 = H, R5 = N-methylcyclohexylamino, 2-MeOC6H4NPr). Although opiate-like, attempts to modify this activity with various substituents have failed to produce antagonistic properties. Some I show

long lasting serotonin antagonism in the guinea pig serotonin toxicity test and the DL-5-hydroxytryptophan induced heat-twitch model in the mouse.

AN 2003:42107 CAPLUS  
 DN 138:89689  
 TI Preparation of 1-phenylethylpiperidines as analgesics  
 IN Sundermann, Bernd; Hoenen, Lambert; Buschmann, Helmut; Koegel,  
 Babette-Yvonne; Friderichs, Elmar  
 PA Gruenenthal G.m.b.H., Germany  
 SO PCT Int. Appl., 54 pp.  
 CODEN: PIXXD2

DT Patent  
 LA German

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003004026	A1	20030116	WO 2002-EP7379	20020703
	W:				
	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,				
	CO, CR, CU, CZ, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM,				
	HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS,				
	LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL,				
	PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA,				
	UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW:				
	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,				
	CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,				
	PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR,				
	NE, SN, TD, TG				
	DE 10132746	A1	20030206	DE 2001-10132746	20010705
	EP 1406623	A1	20040414	EP 2002-745424	20020703
	R:				
	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,				
	IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
	US 2004171640	A1	20040902	US 2004-751584	20040105
PRAI	DE 2001-10132746	A	20010705		
	WO 2002-EP7379	W	20020703		

OS MARPAT 138:89689

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d hitstr

L9 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN  
 IT 484034-05-1P, 2-(1-Phenethylpiperidin-4-yl)-N-phenylacetamide  
 484034-07-3P, N-(2-Methoxyphenyl)-2-(1-phenethylpiperidin-4-yl)acetamide 484034-08-4P, N-(4-Methoxyphenyl)-2-(1-phenethylpiperidin-4-yl)acetamide 484034-09-5P, 2-(1-Phenethylpiperidin-4-yl)-N-(2-trifluoromethoxyphenyl)acetamide 484034-10-8P, N-(3-Methoxyphenyl)-2-(1-phenethylpiperidin-4-yl)acetamide 484034-11-9P, N-(3-Chloro-4-methoxyphenyl)-2-(1-phenethylpiperidin-4-yl)acetamide 484034-12-0P, N-(4-Chloro-2-fluorophenyl)-2-(1-phenethylpiperidin-4-yl)acetamide 484034-13-1P, N-[2-(1-Phenethylpiperidin-4-yl)ethyl]-N-(3-trifluoromethylphenyl)amine 484034-14-2P, N-[2-(1-Phenethylpiperidin-4-yl)ethyl]-N-phenylamine 484034-15-3P, N-(4-Methoxyphenyl)-N-[2-(1-phenethylpiperidin-4-yl)ethyl]amine 484034-17-5P, 2-[[2-(1-Phenethylpiperidin-4-yl)ethyl]amino]phenol 484034-18-6P, 2-(1-Phenethylpiperidin-4-yl)-N-(3-trifluoromethylphenyl)acetamide 484034-19-7P, (3-Methoxyphenyl)-[2-(1-phenethylpiperidin-4-yl)ethyl]amine 484034-20-0P, (4-Chloro-2-fluorophenyl)-[2-(1-phenethylpiperidin-4-yl)ethyl]amine 484034-21-1P, 4-[[2-(1-Phenethylpiperidin-4-yl)ethyl]amino]phenol 484034-22-2P, 3-[[2-(1-Phenethylpiperidin-4-yl)ethyl]amino]phenol 484034-23-3P, N-(3-Chloro-4-methoxyphenyl)-N-[2-(1-phenethylpiperidin-4-yl)ethyl]acetamide 484034-24-4P, N-(3-Chloro-4-methoxyphenyl)-N-[2-(1-phenethylpiperidin-4-yl)ethyl]propionamide 484034-25-5P,

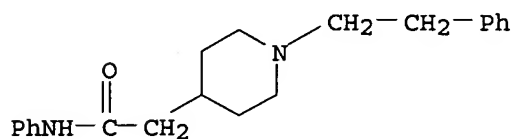
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RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of phenylethylpiperidines as analgesics)

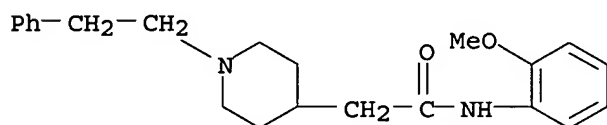
RN 484034-05-1 CAPLUS

CN 4-Piperidineacetamide, N-phenyl-1-(2-phenylethyl)- (9CI) (CA INDEX NAME)



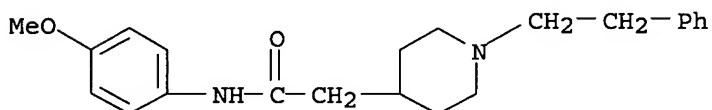
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CN 4-Piperidineacetamide, N-(2-methoxyphenyl)-1-(2-phenylethyl)- (9CI) (CA INDEX NAME)



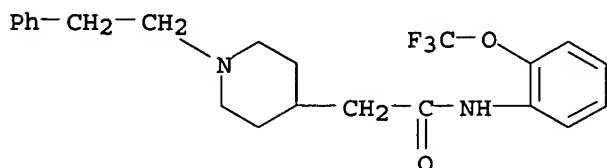
RN 484034-08-4 CAPLUS

CN 4-Piperidineacetamide, N-(4-methoxyphenyl)-1-(2-phenylethyl)- (9CI) (CA INDEX NAME)



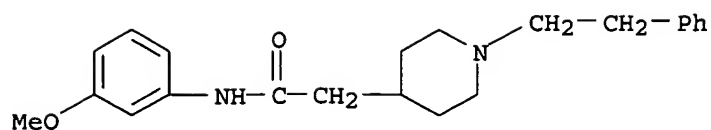
RN 484034-09-5 CAPLUS

CN 4-Piperidineacetamide, 1-(2-phenylethyl)-N-[2-(trifluoromethoxy)phenyl]- (9CI) (CA INDEX NAME)



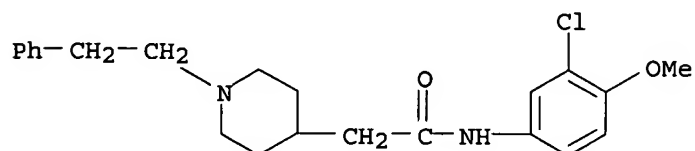
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CN 4-Piperidineacetamide, N-(3-methoxyphenyl)-1-(2-phenylethyl)- (9CI) (CA INDEX NAME)



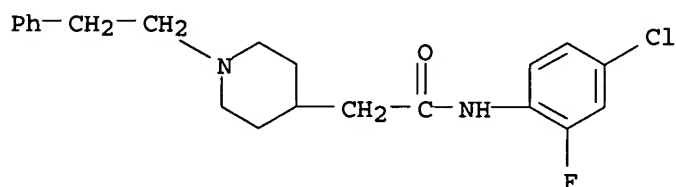
RN 484034-11-9 CAPLUS

CN 4-Piperidineacetamide, N-(3-chloro-4-methoxyphenyl)-1-(2-phenylethyl)-  
(9CI) (CA INDEX NAME)



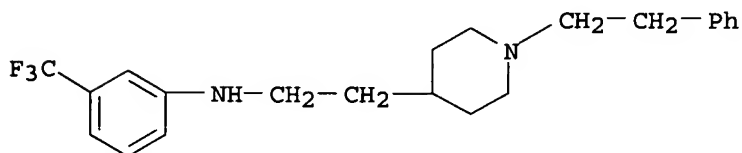
RN 484034-12-0 CAPLUS

CN 4-Piperidineacetamide, N-(4-chloro-2-fluorophenyl)-1-(2-phenylethyl)-  
(9CI) (CA INDEX NAME)



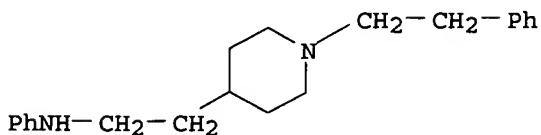
RN 484034-13-1 CAPLUS

CN 4-Piperidineethanamine, 1-(2-phenylethyl)-N-[3-(trifluoromethyl)phenyl]-  
(9CI) (CA INDEX NAME)



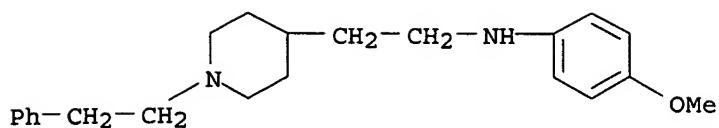
RN 484034-14-2 CAPLUS

CN 4-Piperidineethanamine, N-phenyl-1-(2-phenylethyl)- (9CI) (CA INDEX NAME)

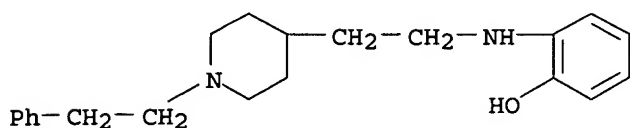


RN 484034-15-3 CAPLUS

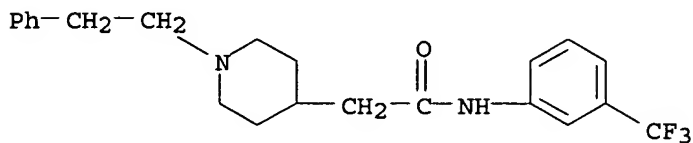
CN 4-Piperidineethanamine, N-(4-methoxyphenyl)-1-(2-phenylethyl)- (9CI) (CA INDEX NAME)



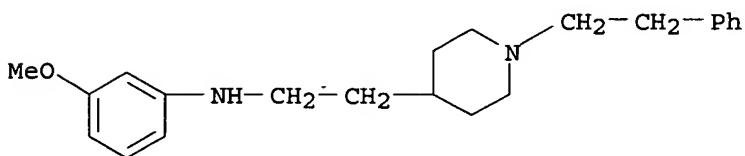
RN 484034-17-5 CAPLUS  
 CN Phenol, 2-[[2-[1-(2-phenylethyl)-4-piperidinyl]ethyl]amino]- (9CI) (CA INDEX NAME)



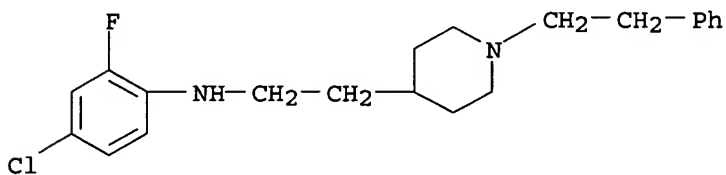
RN 484034-18-6 CAPLUS  
 CN 4-Piperidineacetamide, 1-(2-phenylethyl)-N-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



RN 484034-19-7 CAPLUS  
 CN 4-Piperidineethanamine, N-(3-methoxyphenyl)-1-(2-phenylethyl)- (9CI) (CA INDEX NAME)

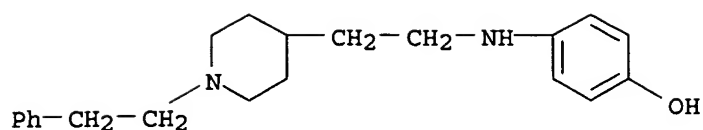


RN 484034-20-0 CAPLUS  
 CN 4-Piperidineethanamine, N-(4-chloro-2-fluorophenyl)-1-(2-phenylethyl)- (9CI) (CA INDEX NAME)

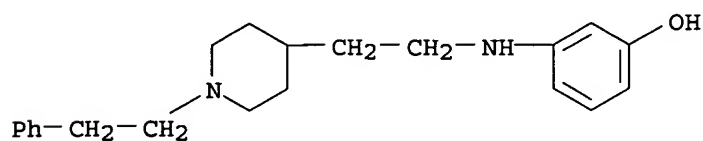


RN 484034-21-1 CAPLUS  
 CN Phenol, 4-[[2-[1-(2-phenylethyl)-4-piperidinyl]ethyl]amino]- (9CI) (CA INDEX NAME)

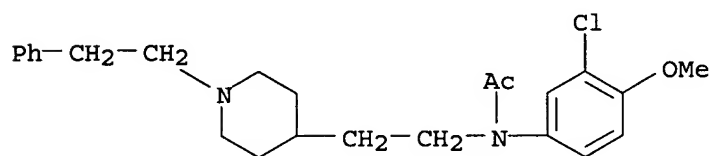




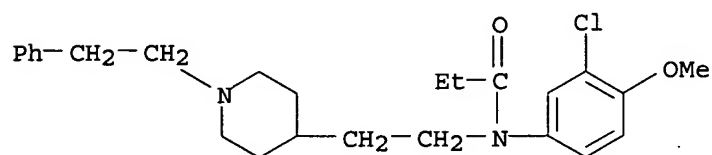
RN 484034-22-2 CAPLUS  
 CN Phenol, 3-[[2-[1-(2-phenylethyl)-4-piperidinyl]ethyl]amino] - (9CI) (CA INDEX NAME)



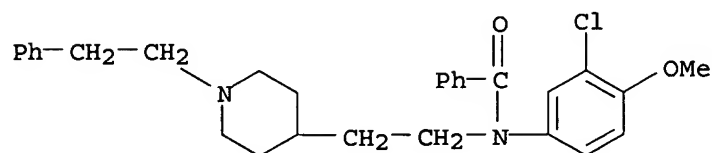
RN 484034-23-3 CAPLUS  
 CN Acetamide, N-(3-chloro-4-methoxyphenyl)-N-[2-[1-(2-phenylethyl)-4-piperidinyl]ethyl] - (9CI) (CA INDEX NAME)



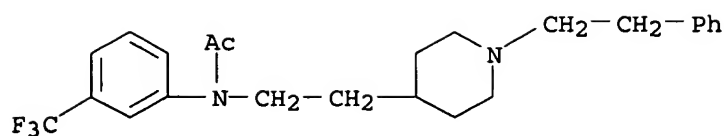
RN 484034-24-4 CAPLUS  
 CN Propanamide, N-(3-chloro-4-methoxyphenyl)-N-[2-[1-(2-phenylethyl)-4-piperidinyl]ethyl] - (9CI) (CA INDEX NAME)



RN 484034-25-5 CAPLUS  
 CN Benzamide, N-(3-chloro-4-methoxyphenyl)-N-[2-[1-(2-phenylethyl)-4-piperidinyl]ethyl] - (9CI) (CA INDEX NAME)

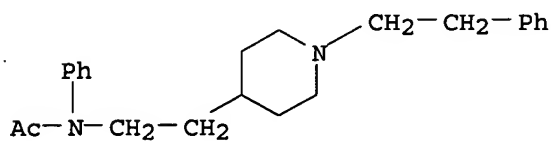


RN 484034-27-7 CAPLUS  
 CN Acetamide, N-[2-[1-(2-phenylethyl)-4-piperidinyl]ethyl]-N-[3-(trifluoromethyl)phenyl] - (9CI) (CA INDEX NAME)



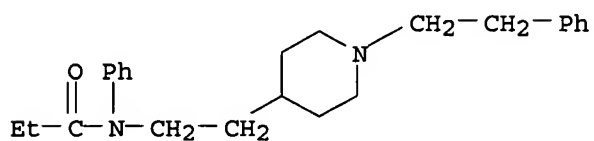
RN 484034-28-8 CAPLUS

CN Acetamide, N-phenyl-N-[2-[1-(2-phenylethyl)-4-piperidinyl]ethyl]- (9CI)  
(CA INDEX NAME)



RN 484034-29-9 CAPLUS

CN Propanamide, N-phenyl-N-[2-[1-(2-phenylethyl)-4-piperidinyl]ethyl]- (9CI)  
(CA INDEX NAME)



RN 484034-30-2 CAPLUS

CN Benzamide, N-phenyl-N-[2-[1-(2-phenylethyl)-4-piperidinyl]ethyl]- (9CI)  
(CA INDEX NAME)

